Chemical Structure and Orientation of Ethylene

on Si(114)-
$$(2\times1)/c(2\times2)$$

D. E. Barlow, S.C. Erwin, A. R. Laracuente, L. J. Whitman, and J. N. Russell, Jr.*

Naval Research Laboratory

Chemistry Division

4555 Overlook Ave., SW

Washington, DC 20375-5342

SUPPORTING INFORMATION

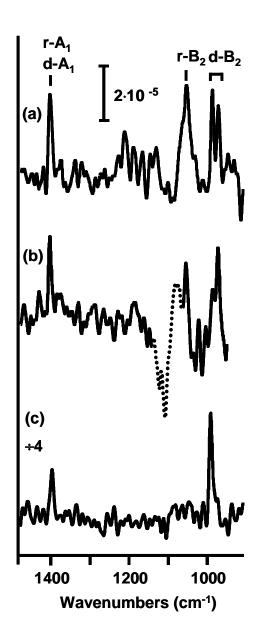


Figure S1. Comparison of low frequency modes for ethylene di-sigma bonded to dimers and/or rebonded atoms. (a) 0.37 ML ethylene-Si(114); (b) 0.27 ML ethylene-Si(114); The dotted portion of the spectrum indicates miscancellation of a Si phonon

mode and is not related to ethylene adsorption. (c) 0.35 ML ethylene-Si(001). All spectra were acquired without a polarizer using an MCT-B detector.

The labels "r-A₁" and "d-A₁" in Figure S1 identify the assigned position for the ethylene-rebonded atom and ethylene-dimer A₁ C-C stretch + C-H wag. In the ethylene-Si(114) spectra, these two modes are apparently unresolved and observed as a single peak. (Only the d-A₁ mode will be observed in the ethylene-Si(001) spectrum.) The "r-B₂" and "d-B₂" labels identify the assigned peaks for the ethylene-rebonded atom and ethylene-dimer B₂ rocking modes, respectively. Note that the r-B₂ peak is observed only in the ethylene-Si(114) spectra, as expected. The higher frequency shoulders on the r-B₂ peaks are due to Si phonon miscancellations.

Two peaks are observed in the d-B₂ region of the ethylene-Si(114) spectra. At this point, we have not identified the origin of the two peaks, however there does appear to be a coverage dependence of the relative intensities. At the 0.27 ML coverage, the lower frequency peak has the highest intensity. As the ethylene coverage is increased, the low frequency peak decreases in intensity while the higher frequency peak intensity increases. The ethylene-Si(001) system also exhibits coverage dependent behavior in this region. We are currently working to identify the origin of this trend.